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Moment quantization and (A-adic) discrete–continuous wavelet transform theory

C R Handy and R Murenzi

Department of Physics and Center for Theoretical Studies of Physical Systems, Clark Atlanta University, Atlanta, GA 30314, USA

Abstract. We establish how moment quantization directly leads to a complete (A-adic) discrete–continuous wavelet transform theory in contrast to the approximate reconstruction methods published earlier (1996 *Phys. Rev.* A **54** 3754, 1997 *J. Phys. A: Math. Gen.* **30** 4709).

1. Introduction

Wavelet transform theory (Chui 1992) defines an efficient multiscale tool with regards to the *time-frequency* or *space-scale* analysis of images and signals, detection and recognition of objects (Antoine *et al* 1995), and the numerical analysis of many-body quantum systems (Tymczak and Wang 1997). Whereas Fourier analysis is inappropriate for studying localized (transient) structures, wavelets are specifically well adapted to address such problems ever since the formulation by Grossmann and Morlet (1984). These general observations apply to all three types of wavelet formalisms: (i) the continuous wavelet transform (CWT); (ii) the discretization of CWT, to be referred to as DCWT (Daubechies 1991); and (iii) the purely discrete formulation (DWT), as represented through Daubechies' pioneering work with orthnormal wavelets (1988).

Wavelet analysis is an intrinsically multiscale formalism for analysing important, localized, transient effects. An important class of problems that can benefit from such analytical tools are those corresponding to Schrödinger Hamiltonians with strongly coupled interactions, or those requiring semiclassical analysis. These systems are sensitive to the singular perturbation (Bender and Orzag 1978) contributions associated with the underlying turning points (hypersurfaces). Such (multidimensional) problems can be studied through wavelet methods based in part on the formalism presented here (Handy *et al* 1999).

For such types of continuous systems, the corresponding continuous structure of both CWT and DCWT highly recommends them as appropriate analytical/numerical tools. This is a welcomed contribution, since relatively little work had been done, during the formative 'wavelet' years, in incorporating CWT and DCWT into quantum operator theory (Paul 1984, Plantevin 1992). An important limitation had been the overcomplete nature of the underlying wavelet basis and their nonorthogonality. Through the adoption of a moment-based reformulation, one can circumvent these difficulties. In contrast, through the development of discrete orthonormal wavelets, DWT has established itself as a very powerful tool in the multiresolution analysis of discrete systems.

The recent works by Handy and Murenzi (HM) (1996, 1997, 1998a, b, 1999) mark a significant first step in the systematic integration of CWT (and DCWT, as developed in this paper) into quantum mechanics. This has primarily come about through the discovery of the important, complementary, role moment quantization (MQ) (Tymczak *et al* 1998a, b, Handy

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et al 1988a, b) plays in facilitating the incorporation of CWT/DCWT methods in the analysis of Schrödinger operator problems with rational fraction potentials. Almost all physical processes can be described by such potentials (or transformed into such form); therefore, these define a sufficiently broad class of relevant and important problems. For such systems, as established in the very recent work by HM (1998a, b), MQ and CWT are equivalent and inseparable.

The preceding narrative may suggest that MQ is to be defined only through the works cited. However, the broader connotation of MQ, as implied here, is to also refer to all techniques for determining the physical values for the scaled and translated moments $\mu_{a,b}(p) \equiv \int \mathrm{d}x\, x^p \mathcal{G}(\frac{x-b}{a})\Psi(x)$, involving the desired configuration, Ψ, and a specified function, $\mathcal{G}$ (which can either be a scaling function, $\mathcal{S}$, or the generator corresponding to a given *mother wavelet* function, $\mathcal{W} = \partial^i \mathcal{G}$). These are discussed below. For a sufficiently broad class of $\mathcal{G}$-functions, the underlying linear (Schrödinger) differential equation can be transformed into a closed, coupled set of linear (partial) differential equations (with respect to the scale, a, and translation, b, variables) involving the $\mu_{a,b}(p)$. The importance of such moment differential relations had been overlooked by the CWT community, in general, but conveniently exploited in the works by HM.

Given the equivalency between MQ and CWT, as established by HM's earlier works, the major contribution of this work is the extension of this philosophy to the DCWT case as well. From the perspective of MQ, we present an MQ-DCWT formalism that is immediately accessible, and which serves to clarify the approximate nature of previous efforts (HM 1996, 1997), as viewed from the MQ perspective.

In order to facilitate logical progression in this work, we quickly review the essential underlying formalism, and outline the results to be derived.

Let $Q(x) = \sum_{n=0}^{2N} \Xi(n)x^n$ be a given, even degree, polynomial satisfying $\Xi(0) = 1$, and $\Xi(2N) > 0$. Define the scaled ($a > 0$) and translated ($b \in (-\infty, +\infty)$) moments,

$$\mu_{a,b}(p) = \int \mathrm{d}x\, x^p \mathrm{e}^{-Q(\frac{x}{a})}\Psi(x+b) \tag{1.1}$$

of the (unknown) bound state wavefunction, Ψ. According to HM (1996, 1997, 1998a, b, 1999), for one-dimensional Schrödinger potential problems with rational fraction potentials, these moments will satisfy a $(1+m_s)$-dimensional (m_s is problem dependent), linear, first-order coupled differential equation with respect to the inverse scale variable, $\frac{1}{a}$:

$$\partial_{\frac{1}{a}} \vec{\mu}_{a,b} = \mathcal{M}[a, b, E]\vec{\mu}_{a,b} \tag{1.2}$$

where $\vec{\mu}_{a,b} \equiv (\mu_{a,b}(0), \ldots, \mu_{a,b}(m_s))$. The matrix $\mathcal{M}[a, b, E]$ is readily determinable and depends on the energy variable, E, as well. The moments involved in equation (1.2) are referred to as the *missing moments*. These coupled equations define an initial value problem in which knowledge of the physical values for $\vec{\mu}_{\infty,b}$ and E enable the generation of all moments, for all scale and translation parameter values. The $\vec{\mu}_{\infty,b}$ and E are determined through MQ analysis.

In the zero-scale limit, the asymptotic behaviour of the moments can be used to recover $\Psi(b)$:

$$\mathrm{Lim}_{a\to 0}\mu_{a,b}(p) = a^{1+p}\nu(p)\Psi(b) \tag{1.3}$$

provided $\nu(p) \equiv \int \mathrm{d}x\, x^p \mathrm{e}^{-Q(x)} \neq 0$. This procedure yields excellent pointwise results (HM 1996, 1997, 1998a, b, 1999). However, it does not offer a manifestly global representation of the underlying multiscale contributions that generate the local, pointwise, structure of Ψ (as represented in Daubechies' dyadic expansion in equation (1.9), or the alternative DCWT representation derived in section 3). This is where wavelets make an important contribution.

The above formalism is manifestly non-wavelet. However, it has been shown (HM 1998a, b) (and briefly rederived in section 3) that asymptotic moment limits of the above type correspond exactly to the CWT signal-wavelet inversion formula:

$$\Psi(b) = \frac{1}{\nu}\int_0^{+\infty}\frac{\mathrm{d}a}{a^{\frac{5}{2}}}\int_{-\infty}^{+\infty}\mathrm{d}\xi\,\mathcal{D}\left(\frac{\xi-b}{a}\right)W\Psi(a,\xi) \tag{1.4}$$

where the wavelet transform is defined by

$$W\Psi(a,\xi) = \frac{1}{\sqrt{a}}\int_{-\infty}^{+\infty}\mathrm{d}x\,\mathcal{W}\left(\frac{x-\xi}{a}\right)\Psi(x) \tag{1.5}$$

involving a suitable *mother* wavelet function, $\mathcal{W}(x)$, with corresponding dual: $\mathcal{D}(x)$.

In terms of their Fourier transforms (i.e. $\hat{\mathcal{W}}(k) = \frac{1}{\sqrt{2\pi}}\int \mathrm{d}k\,\mathrm{e}^{-\mathrm{i}kx}\mathcal{W}(x)$, etc) the mother wavelet and dual are acceptable so long as the product of their Fourier transforms satisfy the relation,

$$-k\partial_k\hat{\mathcal{S}}(k) = \sqrt{2\pi}\hat{\mathcal{W}}(k)\hat{\mathcal{D}}(k) \tag{1.6}$$

where $\mathcal{S}$ is an arbitrary well-behaved, integrable function that must satisfy $\nu \equiv \int \mathrm{d}x\,S(x) \neq 0$. So long as $\mathcal{W}$ and $\mathcal{D}$ define a satisfactory *scaling function*, $\mathcal{S}$, equation (1.4) holds. Different choices of scaling functions will affect the integrability characterstic of equation (1.4) (refer to the discussion following equation (3.2) for clarification of this point).

All of the problems studied by HM use special, infinitely differentiable, scaling functions whose closed-form structure allowed them to bypass the explicit consideration of mother wavelet and dual functions. However, in principle, faster recovery of $\Psi(b)$ can be achieved by selecting a mother wavelet and dual function whose associated scaling function may not have the aforementioned 'nice' properties (i.e. finitely differentiable and/or not obtainable in closed form, etc). In such cases, the HM formalism can only generate the wavelet transform, which must then be integrated through the inversion relation given in equation (1.4). The two-dimensional integration character, of such an inversion procedure is numerically unattractive and motivates the desire to obtain an equivalent DCWT formalism, as presented in this work.

If one regards the translated and scaled copies of the dual function as a basis,

$$\mathcal{B} = \left\{\mathcal{D}\left(\frac{\xi-b}{a}\right)|a>0,|b|<\infty\right\} \tag{1.7}$$

it is overcomplete, since different choices of mother wavelets, $\mathcal{W}_i$, lead to different sets of wavelet transform coefficients, $\{W_i\Psi(a,\xi)|a > 0,|\xi| < \infty\}$, each generating the same configuration, Ψ.

Many of the popular mother wavelets correspond to expressions of the type $\mathcal{W}(x) = \mathcal{N}\partial_x^i\mathrm{e}^{-Q(x)} = \sum_{j=0}^{J}\mathcal{C}_j x^j\mathrm{e}^{-Q(x)}$, for $i \geqslant 1$, and $Q(x)$ as defined previously. It then follows that the wavelet transform is a linear superposition of the moments

$$W\Psi(a,b) = \frac{1}{\sqrt{a}}\sum_{j=0}^{J}\frac{\mathcal{C}_j}{a^j}\mu_{a,b}(j). \tag{1.8}$$

For rational fraction potential problems, the moments $\{\mu_{a,b}(p)|p \geqslant 1+m_s\}$ linearly depend on the *missing* moments, $\{\mu_{a,b}(\ell)|0 \leqslant \ell \leqslant m_s\}$. Once the latter are determined through MQ analysis and integration of equation (1.2), all of the moments, for a given scale and translation, (a,b), are determined, as well as the wavelet transform, $W\Psi(a,b)$.

Knowledge of the wavelet transform allows us to view equation (1.4) as a global representation of the multiscale contributions definining the local structure of Ψ at b. However, the continuous two-dimensional structure of this integral representation can make any ensuing analysis difficult. For this reason, the realization of a discretized analogue is important. To this

extent, the works by HM cite Daubechies' dyadic approximation, for the *Mexican hat* mother wavelet and dual, $\mathcal{W}_h(x) = \mathcal{D}_h(x) = -\mathcal{N}_h \partial_x^2 \mathrm{e}^{-\frac{x^2}{2}}$ where $\mathcal{N}_h \equiv \frac{2}{\sqrt{3\sqrt{\pi}}}$:

$$\Psi(x) \approx \frac{2}{6.819} \sum_{l,j} \mathcal{W}_{l,j} \frac{1}{\sqrt{2^l}} \mathcal{W}_h \left(\frac{x - j2^l}{2^l} \right) \tag{1.9}$$

where $\mathcal{W}_{l,j} \equiv W\Psi(2^l, j2^l)$.

The structure of this relation is very appealing, since it suggests that the dyadic copies of the (wavelet) dual define a basis. However, the limited use of this dyadic formula failed to yield as good a convergence to $\Psi(b)$ as did the integration of equation (1.2) combined with the asymptotic formulae in equation (1.3). Indeed, from an MQ perspective, equation (1.9) is an approximation to the exact expression. Refer to the discussion pertaining to equation (3.21).

We clarify this important point. Let $\mathrm{Re} \subset (0, \infty) \times (-\infty, +\infty)$ denote the subset of the (a, b) wavelet transform parameter space within which the Runge–Kutta (RK) integration of equation (1.2) is numerically stable. Then HM's investigations showed that the generated $\mathcal{W}_{l,j}$ wavelet coefficients corresponding to $(a = 2^l, b = j2^l) \in \mathrm{Re}$, for a limited range of (l, j) values, did not reproduce the quantum configuration states as well as the asymptotic estimates corresponding to equation (1.3). In order to better understand a possible source for this discrepancy, we were motivated to understand (from the MQ perspective) the exact structure of the DCWT representation for equation (1.4).

One of the results of this work is the derivation of the exact DCWT representation of equation (1.4), from the MQ perspective. This is done in section 3 (refer to either equation (3.19*b*), (3.20), or (3.22)). The DCWT formulation to be presented yields comparable results to those published previously by HM, when used to the same expansion order, and improves upon these when the expansion order is increased (i.e. when greater l values are allowed). This is discussed in section 4.

2. Moment-wavelet quantization

In this section we develop more fully some of the key concepts essential to this work. The technical details are given in the cited references.

The multiscale efficiency of wavelets derives from its key objective: to understand the interplay between 'dynamical' structures at different scales, particularly in terms of how larger-scale effects impact smaller-scale behaviour. A simple relation that captures the essence of this is the generalized moment expression:

$$\mathcal{U}_{a,b} \equiv \frac{1}{\nu} \int \mathrm{d}x \, \mathcal{S}\left(\frac{x - b}{a} \right) \Psi(x) \tag{2.1}$$

involving the (unknown) bound state wavefunction, Ψ, and a sufficiently well-behaved kernel ('scaling') function, $\mathcal{S}$, satisfying $\nu \equiv \int \mathrm{d}x \, \mathcal{S}(x) \neq 0$ and $|\nu| < \infty$. The scale and translation parameters are $a > 0$ and $b \in (-\infty, +\infty)$, respectively. In the small-scale (continuum) limit, we have

$$\mathrm{Lim}_{a \to 0} \frac{\mathcal{U}_{a,b}}{a} = \Psi(b). \tag{2.2}$$

As previously noted, this simple asymptotic relation directly leads (and is equivalent) to the standard signal-wavelet CWT reconstruction formula in equation (1.4).

We may view equation (2.2) as an analytical microscope by which the pointwise behaviour of $\Psi(b)$ is generated through successive 'fine tuning' of the scale parameter variable defining

$\mathcal{U}_{a,b}$, starting at $a = \infty$ and proceeding to $a = 0$. These types of expressions were studied, in a similar context, almost 20 years ago by Handy (1981).

In order to understand the interplay between the various scales (i.e. how effects at scale 'a' affect things at smaller scales, $a' < a$), it is natural to study the differential expressions

$$\partial_a \mathcal{U}_{a,b} = -\frac{1}{\nu a^2} \int \mathrm{d}x\, (x-b) \mathcal{S}^{(1)} \left(\frac{x-b}{a} \right) \Psi(x) \tag{2.3a}$$

$$\partial_b \mathcal{U}_{a,b} = -\frac{1}{\nu a} \int \mathrm{d}x\, \mathcal{S}^{(1)} \left(\frac{x-b}{a} \right) \Psi(x) \tag{2.3b}$$

and their higher-order generalization, $\partial_a^m \partial_b^n \mathcal{U}_{a,b}$, which involve the summation of integrand terms of the form $(x-b)^p \mathcal{S}^{(q)}(\frac{x-b}{a})$, (i.e. $\partial_x^q \mathcal{S} \equiv \mathcal{S}^{(q)}$) for varying combinations of p and q.

Relating all of these differential expressions is greatly simplified if the scaling function satisfies

$$\partial_x^n \mathcal{S}(x) = \mathcal{P}_n(x) \mathcal{S}(x) \tag{2.4}$$

where $\mathcal{P}_n(x)$ is a polynomial (i.e. $\mathcal{S}(x) = \mathrm{e}^{-Q(x)}$, for an appropriate polynomial, Q). Under this assumption, it is then sufficient to consider the multiscale interactions of the generalized moments

$$\mu_{a,b}(p) \equiv \int \mathrm{d}x\, x^p \mathcal{S}\left(\frac{x}{a} \right) \Psi(x+b). \tag{2.5}$$

In the infinite-scale limit, $a \to \infty$, these converge to finite sums involving the moments:

$$\mathrm{Lim}_{a \to \infty}\, \mu_{a,b}(p) = \mu_{\infty,b}(p) = \sum_{\rho=0}^{p} \binom{p}{\rho} (-b)^{p-\rho} \mu(\rho) \tag{2.6}$$

where $\binom{p}{\rho} \equiv \frac{p!}{(p-\rho)!\rho!}$ and $\mu(\rho) \equiv \int \mathrm{d}x\, x^\rho \Psi(x)$, assuming $S(0) \equiv 1$.

One convenient feature of the $\mu_{a,b}(p)$ is that for a broad class of scaling functions (not just those corresponding to $\mathcal{S}(x) = \mathrm{e}^{-Q(x)}$ where Q is a polynomial), in any space dimension, the moments will satisfy a finite difference equation in 'p', of order $1 + m_s$, that is straightforward to generate and solve through MQ analysis.

Limiting the discussion to one dimension, for simplicity, consider the Schrödinger operator eigenenergy problem

$$-\partial_x^2 \Psi(x) + V(x) \Psi(x) = E \Psi(x) \tag{2.7}$$

where the potential is a rational fraction

$$V(x) = \frac{\sum_{i=0}^{T} \mathcal{N}(i) x^i}{\sum_{j=0}^{B} \mathcal{D}(j) x^j}. \tag{2.8}$$

The configuration $\Phi_{a,b}(x) \equiv \mathrm{e}^{-Q(\frac{x}{a})} \Psi(x+b)$, also satisfies a second-order differential equation

$$-\left(\partial_x^2 \Phi_{a,b}(x) + \frac{2}{a} Q'\left(\frac{x}{a} \right) \partial_x \Phi_{a,b}(x) + \frac{1}{a^2} \left[Q''\left(\frac{x}{a} \right) + \left(Q'\left(\frac{x}{a} \right) \right)^2 \right] \Phi_{a,b}(x) \right) + V(x+b) \Phi_{a,b}(x) = E \Phi_{a,b}(x). \tag{2.9}$$

Through the standard MQ formalism (Tymczak *et al* 1998a, b, Handy *et al* 1988a, b, Handy and Bessis 1985), one can transform this differential equation into a homogeneous, linear finite difference equation of order $1 + m_s$ ($m_s = \mathrm{Max}\{T, B\} - 1$) for the moments of $\Phi_{a,b}(x)$, the $\mu_{a,b}(p)$. As such, the moments $\{\mu_{a,b}(p) | p \geqslant m_s + 1\}$ will be linearly dependent on the first $1 + m_s$ moments (the *missing* moments), $\{\mu_{a,b}(\ell) | 0 \leqslant \ell \leqslant m_s\}$, as represented by

$$\mu_{a,b}(p) = \sum_{\ell=0}^{m_s} M_{a,b,E}(p, \ell) \mu_{a,b}(\ell) \tag{2.10}$$

where $p \geqslant 0$, and the energy, E, dependent M-coefficients are readily obtainable. Self-consistency requires that for the missing moment indices we have: $M_{a,b,E}(\ell_1, \ell_2) = \delta_{\ell_1,\ell_2}$, for $0 \leqslant \ell_1, \ell_2 \leqslant m_s$.

So long as $Q(x)$ (i.e. a rational fraction) grows slower (in any complex x-direction) than the JWKB asymptotic estimate (Bender and Orzag 1978), the $\mu_{a,b}(p)$, will be regular in $\alpha \equiv \frac{1}{a}$, making the integration of equation (1.2) free of any singularities near the origin with respects to the α, inverse scale, independent variable. The case of the Bohr potential (via the Mexican hat wavelet) differs from this, as discussed in HM (1997).

Taking all the above into account, and further restricting $Q(x)$ to be an even degree polynomial, $Q(x) = \sum_{n=0}^{2N} \Xi(n) x^n$, we obtain equation (1.2) as follows. Consider the first-order derivative relations (note that $\mu_{\alpha,b}(p) \equiv \mu_{a(\alpha),b}(p)$):

$$\partial_\alpha \mu_{\alpha,b}(p) = \partial_\alpha \int \mathrm{d}x\, x^p \mathrm{e}^{-Q(\alpha x)} \Psi(x+b) \tag{2.11a}$$

or

$$\partial_\alpha \mu_{\alpha,b}(p) = -\int \mathrm{d}x\, x^{p+1} Q'(\alpha x) \mathrm{e}^{-Q(\alpha x)} \Psi(x+b) \tag{2.11b}$$

becoming

$$\partial_\alpha \mu_{\alpha,b}(p) = -\sum_{n=0}^{2N} n\alpha^{n-1} \Xi(n) \mu_{\alpha,b}(p+n). \tag{2.11c}$$

From equation (2.10), upon making the appropriate substitution, $\mu_{\alpha,b}(p+n) = \sum_{\ell=0}^{m_s} M_{\alpha,b,E}(p+n, \ell) \mu_{\alpha,b}(\ell)$, we obtain

$$\partial_\alpha \mu_{\alpha,b}(p) = \sum_{\ell=0}^{m_s} \left(-\sum_{n=0}^{2N} n\alpha^{n-1} \Xi(n) M_{\alpha,b,E}(p+n, \ell) \right) \mu_{\alpha,b}(\ell). \tag{2.12}$$

Restricting $0 \leqslant p \leqslant m_s$, we obtain (i.e. equation (1.2))

$$\partial_\alpha \begin{pmatrix} \mu_{\alpha,b}(0) \\ \mu_{\alpha,b}(1) \\ \cdot \\ \cdot \\ \cdot \\ \mu_{\alpha,b}(m_s) \end{pmatrix} = \begin{pmatrix} \mathcal{M}_{0,0}[\alpha, b, E] \cdots \mathcal{M}_{0,m_s}[\alpha, b, E] \\ \mathcal{M}_{1,0}[\alpha, b, E] \cdots \mathcal{M}_{1,m_s}[\alpha, b, E] \\ \cdots \\ \cdots \\ \cdots \\ \mathcal{M}_{m_s,0}[\alpha, b, E] \cdots \mathcal{M}_{m_s,m_s}[\alpha, b, E] \end{pmatrix} \begin{pmatrix} \mu_{\alpha,b}(0) \\ \mu_{\alpha,b}(1) \\ \cdot \\ \cdot \\ \cdot \\ \mu_{\alpha,b}(m_s) \end{pmatrix} \tag{2.13}$$

where the $\mathcal{M}_{\ell_1,\ell_2}[\alpha, b, E]$ matrix elements are defined through equation (2.12).

Utilizing any of the various MQ formalisms (Handy 1999a, Handy *et al* 1999, Tymczak *et al* 1998a, b, Handy *et al* 1988a, b, Killingbeck *et al* 1985, Handy and Bessis 1985, Blankenbecler *et al* 1980), we can determine the physical bound state energy and corresponding (infinite-scale) missing moments, $E, \{\mu(\ell) | \ell \leqslant m_s\}$, respectively. Through equation (2.6), these missing moments can be used to determine the infinite-scale missing moments at point b, $\{\mu_{\alpha=0,b}(\ell) | \ell \leqslant m_s\}$. In this manner, we can integrate equation (2.13), and through equation (2.2) recover the pointwise structure of the bound state configuration, $\Psi(b)$. More generally, so long as $\nu(p) \equiv \int \mathrm{d}x\, x^p \mathcal{S}(x) \neq 0$, one has a larger number of asymptotic relations through which to recover $\Psi(b)$:

$$\mathrm{Lim}_{\alpha\to\infty}(\alpha^{p+1} \mu_{\alpha,b}(p)) = \nu(p) \Psi(b). \tag{2.14}$$

It is also possible to determine the energy and missing moment values directly from equation (2.13), this is discussed elsewhere (Handy 1999b, Handy *et al* 1999).

We will use the above formalism to generate the wavelet transform coefficients for the dyadic scale and translation parameter values required in the MQ-DCWT reconstruction formula(e) derived in the following section.

3. Deriving the CWT/DCWT inversion formulae

3.1. The CWT transform and its inverse

As noted in the previous sections, the asymptotic relation in equation (1.3), or equation (2.14), yields a pointwise convergent formalism for recovering the physical wavefunction configuration. This approach works very well, as documented in the various cited works by HM. We want to generate a global reconstruction formalism which manifestly incorporates the multiscale features inherent to the representation in equation (1.3). We briefly review the derivation of the inverse CWT transform formula given by HM (1998a, b). We will use this in motivating the inverse DCWT transform formula(e) derived in section 3.2.

Consider the generalized, affine (convolution) transform, of a configuration $\Psi(x)$

$$U_{\mathcal{S}}[a,b] \equiv \frac{1}{\nu}\int_{-\infty}^{\infty}\frac{\mathrm{d}x}{a}\mathcal{S}\left(\frac{x-b}{a}\right)\Psi(x). \tag{3.1}$$

Note that $U_{\mathcal{S}}[a,b] = \frac{1}{a}\mathcal{U}_{a,b}$, as defined in equation (2.1).

The scaling function, $\mathcal{S}$, is arbitrary, provided it is integrable and its zeroth-order moment is nonzero ($\nu \equiv \nu(0) \neq 0$). Also, for our purposes, it must be differentiable. The zero-scale limit becomes

$$\mathrm{Lim}_{a\to 0}U_{\mathcal{S}}[a,b] = \Psi(b). \tag{3.2}$$

Clearly, this relation emulates the Dirac integral $\int \mathrm{d}x\,\delta(x-b)\Psi(x)$. The rate of convergence is determined by the choice of $\mathcal{S}$. Generally, faster convergence to Ψ is determined by the extent to which $\nu(i) = \int \mathrm{d}x\,x^i\mathcal{S}(x) = 0$, for $1 \leqslant i \leqslant I$. The greater is '$I$', the faster is the convergence. This is readily apparent upon shifting by $x \to x + b$, performing the change of variables $y = \frac{x}{a}$, and expanding $\Psi(b + ay) = \sum_{i=0}\frac{\Psi^{(i)}(b)(ay)^i}{i!}$, all within the integral for $U_{\mathcal{S}}[a,b]$.

We can rewrite equation (3.2) as

$$-\int_0^{\infty}\mathrm{d}a\,\partial_a U_{\mathcal{S}}[a,b] = \Psi(b) \tag{3.3}$$

since $U_{\mathcal{S}}[\infty,b] = 0$. Substituting equation (3.1) yields

$$\Psi(b) = \frac{1}{\nu}\int_0^{\infty}\frac{\mathrm{d}a}{a^2}\int_{-\infty}^{\infty}\mathrm{d}x\,\mathcal{F}\left(\frac{x-b}{a}\right)\Psi(x) \tag{3.4}$$

where $a^{-2}\mathcal{F}(\frac{x-b}{a}) = -\partial_a[\frac{1}{a}\mathcal{S}(\frac{x-b}{a})] = a^{-2}\{\mathcal{S}(\frac{x-b}{a}) + \frac{x-b}{a}\mathcal{S}'(\frac{x-b}{a})\}$, or

$$\mathcal{F}(z) = \partial_z[z\mathcal{S}(z)]. \tag{3.5}$$

The relation in equation (3.4) only integrates over all scales. In order to obtain a result which also integrates over all translations, one must rewrite $\mathcal{F}$ as a convolution integral:

$$\mathcal{F}\left(\frac{x-b}{a}\right) = \int_{-\infty}^{\infty}\frac{\mathrm{d}\xi}{a}\,\mathcal{W}\left(\frac{x-\xi}{a}\right)\mathcal{D}\left(\frac{\xi-b}{a}\right) \tag{3.6}$$

(note the rhs $= \int_{-\infty}^{\infty}\frac{\mathrm{d}\xi}{a}\mathcal{D}(\frac{x-\xi}{a})\mathcal{W}(\frac{\xi-b}{a})$) for arbitrary $\mathcal{W}$ and $\mathcal{D}$, provided the respective Fourier transforms satisfy

$$\hat{\mathcal{F}}(k) = \sqrt{2\pi}\hat{\mathcal{W}}(k)\hat{\mathcal{D}}(k). \tag{3.7}$$

Inserting equation (3.6) into (3.4) results in

$$\Psi(b) = \frac{1}{\nu}\int_0^{\infty}\frac{\mathrm{d}a}{a^{\frac{5}{2}}}\int_{-\infty}^{\infty}\mathrm{d}\xi,\mathcal{D}\left(\frac{\xi-b}{a}\right)W\Psi(a,\xi) \tag{3.8a}$$

where

$$W\Psi(a,\xi) \equiv \frac{1}{\sqrt{a}} \int_{-\infty}^{\infty} \mathcal{W}\left(\frac{x-\xi}{a}\right) \Psi(x) \tag{3.8b}$$

denotes the wavelet transform of Ψ.

Combining equations (3.5) and (3.7) one obtains

$$-k\partial_k \hat{\mathcal{S}}(k) = \sqrt{2\pi}\ \hat{\mathcal{W}}(k)\hat{\mathcal{D}}(k) \tag{3.9}$$

as cited earlier. Note that $\hat{\mathcal{F}}(0) = 0$, from equation (3.5); consequently, one assumes that $\hat{\mathcal{W}}(0) = 0$.

3.2. The DCWT inversion algorithm

The first important observation in defining a discretized counterpart to equation (3.8) is to define a general partitioning for equation (3.3):

$$\Psi(b) = \sum_l (U_{\mathcal{S}}[a_l, b] - U_{\mathcal{S}}[a_{l+1}, b]) \tag{3.10}$$

where $-\infty < l < +\infty$, and $a_l \leqslant a_{l+1}$. Thus, $\mathrm{Lim}_{l\to-\infty} a_l = 0^+$, and $\mathrm{Lim}_{l\to+\infty} a_l = +\infty$.

In terms of the kernel $\mathcal{S}$ the above partition becomes

$$\Psi(b) = \frac{1}{v} \sum_l \int_{-\infty}^{+\infty} \mathrm{d}x \left(\frac{1}{a_l}\mathcal{S}\left(\frac{x-b}{a_l}\right) - \frac{1}{a_{l+1}}\mathcal{S}\left(\frac{x-b}{a_{l+1}}\right)\right) \Psi(x). \tag{3.11}$$

We have implicitly assumed the variable 'b' to be arbitrary. At the lth scale value, 'a_l', let us define the representation

$$b = n_l[b]\Delta_l + \delta_l[b] \tag{3.12}$$

($|\frac{\delta_l[b]}{\Delta_l}| < 1$), where Δ_l is some suitable sequence of non-negative values (to be determined), and $n_l[b]$ an appropriate integer expression.

Let us now conjecture that for each a_l scale we have

$$\left(\frac{1}{a_l}\mathcal{S}\left(\frac{x-b}{a_l}\right) - \frac{1}{a_{l+1}}\mathcal{S}\left(\frac{x-b}{a_{l+1}}\right)\right) = \sum_{j=-\infty}^{+\infty} \mathcal{D}(n_l[b]-j)\ \mathcal{W}_l(x - \xi_b^{(l)}(j)) \tag{3.13}$$

involving the linear function, $\xi_b^{(l)}(j) = \Delta_l \times j + \delta_l[b]$, as well as the (to be specified) discrete function, $\mathcal{D}(j)$, and the continuous functions $\mathcal{W}_l(x)$.

In order to assess the validity of these relations for each 'l', we first transform them into their Fourier space equivalent:

$$\mathrm{e}^{-\mathrm{i}kb}(\hat{\mathcal{S}}(a_l k) - \hat{\mathcal{S}}(a_{l+1}k)) = \sum_{j=-\infty}^{\infty} \mathcal{D}(n_l[b]-j)\hat{\mathcal{W}}_l(k)\mathrm{e}^{-\mathrm{i}k\xi_b^{(l)}(j)} \tag{3.14a}$$

or (upon relabelling the integer summation index)

$$\mathrm{e}^{-\mathrm{i}kb}(\hat{\mathcal{S}}(a_l k) - \hat{\mathcal{S}}(a_{l+1}k)) = \sum_{j=-\infty}^{\infty} \mathcal{D}(j)\hat{\mathcal{W}}_l(k)\mathrm{e}^{-\mathrm{i}k\xi_b^{(l)}(n_l[b]-j)}. \tag{3.14b}$$

Upon substituting $\xi_b^{(l)}(n_l[b]-j) = \Delta_l \times (n_l[b]-j) + \delta_l[b]$, and noting that $b = \Delta_l \times n_l[b] + \delta_l[b]$, equation (3.14$b$) simplifies to

$$(\hat{\mathcal{S}}(a_l k) - \hat{\mathcal{S}}(a_{l+1}k)) = \left[\sum_{j=-\infty}^{\infty} \mathcal{D}(j)\mathrm{e}^{\mathrm{i}kj\Delta_l}\right]\hat{\mathcal{W}}_l(k). \tag{3.15}$$

We can simplify the understanding of equation (3.15) if we define $\rho_l \equiv \frac{a_{l+1}}{a_l} \geqslant 1$ and make the corresponding change of variables, resulting in

$$(\hat{\mathcal{S}}(k) - \hat{\mathcal{S}}(\rho_l k)) = \left[\sum_{j=-\infty}^{\infty} \mathcal{D}(j) \mathrm{e}^{\mathrm{i} \frac{\Delta_l}{a_l} jk} \right] \hat{\mathcal{W}}_l \left(\frac{k}{a_l} \right). \tag{3.16}$$

Since equation (3.16) must hold for all 'l', the simplest choice is to take $\rho_l = \rho > 1$, $\frac{\Delta_l}{a_l} = f$, and $\hat{\mathcal{W}}_l(\frac{k}{a_l}) = \hat{\mathcal{W}}_0(\frac{k}{a_0})$, involving constant ($l$-independent) expressions on the right-hand side. Summarizing these, we have

$$a_l = a_0 \rho^l \tag{3.17a}$$

$$\Delta_l = f a_l = f a_0 \rho^l \tag{3.17b}$$

and

$$\hat{\mathcal{W}}_l(k) = \hat{\mathcal{W}}_0 \left(\frac{a_l}{a_0} k \right) = \hat{\mathcal{W}}_0(\rho^l k) \tag{3.17c}$$

or, in terms of the configuration space transforms:

$$\mathcal{W}_l(x) = \frac{1}{\rho^l} \mathcal{W}_0 \left(\frac{x}{\rho^l} \right). \tag{3.17d}$$

The above equations define the general A-adic representation.

It therefore follows that the only remaining relation to be validated is equation (3.16) rewritten according to the above constraints:

$$(\hat{\mathcal{S}}(k) - \hat{\mathcal{S}}(\rho k)) = \hat{\mathcal{R}}(k) \tag{3.18a}$$

where

$$\hat{\mathcal{R}}(k) \equiv \left[\sum_{j=-\infty}^{\infty} \mathcal{D}(j) \mathrm{e}^{\mathrm{i} f j k} \right] \hat{\mathcal{W}}_0 \left(\frac{k}{a_0} \right). \tag{3.18b}$$

The above relation constrains the three functions $\hat{\mathcal{S}}(k)$, $\hat{\mathcal{W}}_0(k)$, and $\hat{\Upsilon}(k) \equiv \sum_{j=-\infty}^{\infty} \mathcal{D}(j) \mathrm{e}^{\mathrm{i} f j k}$, which is periodic. As in the CWT case, acceptable choices for $\hat{\mathcal{W}}_0$ and $\mathcal{D}(j)$ must generate a scaling function, $\mathcal{S}(x)$, whose zeroth moment is nonzero, $\nu = \int \mathrm{d}x\, \mathcal{S}(x) \neq 0$, and otherwise well behaved (i.e. integrable, Fourier transformable, etc). We shall be working with $\rho = 2$ (i.e. the dyadic case), $f = a_0 = 1$, $\mathcal{D}(j) = -\mathcal{N}_h \partial_j^2 \mathrm{e}^{-\frac{j^2}{2}} = \mathcal{N}_h (1 - j^2) \mathrm{e}^{-\frac{j^2}{2}}$, and $\mathcal{W}_0(x) = -\mathcal{N}_h \partial_x^2 \mathrm{e}^{-\frac{x^2}{2}}$ or $\hat{\mathcal{W}}_0(k) = \mathcal{N}_h k^2 \mathrm{e}^{-\frac{k^2}{2}}$. For this case, the analysis detailed in the appendix yields $\nu \approx 3.427$. In addition, the form of the k-space scaling function is depicted in figures 1 and 2.

3.3. DCWT reconstruction

The DCWT reconstruction of the wavefunction follows upon incorporating equations (3.13) and (3.17) into (3.11) (recall, $b = n_l[b] f a_0 \rho^l + \delta_l(b)$):

$$\Psi(b) = \frac{1}{\nu} \sum_{l=-\infty}^{+\infty} \sum_{j=-\infty}^{+\infty} \mathcal{D}(n_l[b] - j) \int_{-\infty}^{+\infty} \mathrm{d}x\, \mathcal{W}_l(x - \xi_b^{(l)}(j)) \Psi(x) \tag{3.19a}$$

or ($\mathcal{W}_l(x) = \frac{1}{\rho^l} \mathcal{W}_0(\frac{x}{\rho^l})$).

$$\Psi(b) = \frac{1}{\nu} \sum_{l=-\infty}^{+\infty} \sum_{j=-\infty}^{+\infty} \mathcal{D}(n_l[b] - j) \frac{1}{\sqrt{\rho^l}} W\Psi(\rho^l, f a_0 j \rho^l + \delta_l[b]) \tag{3.19b}$$

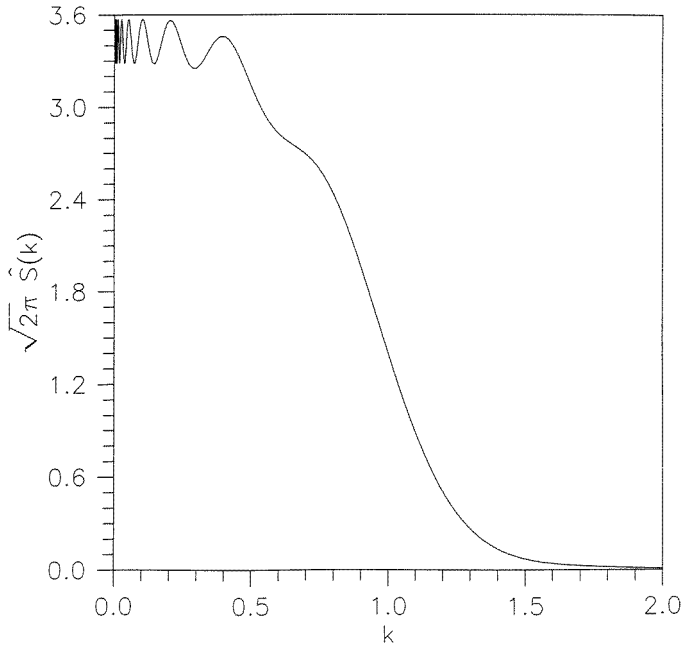

Figure 1. *k*-space plot of scaling function.

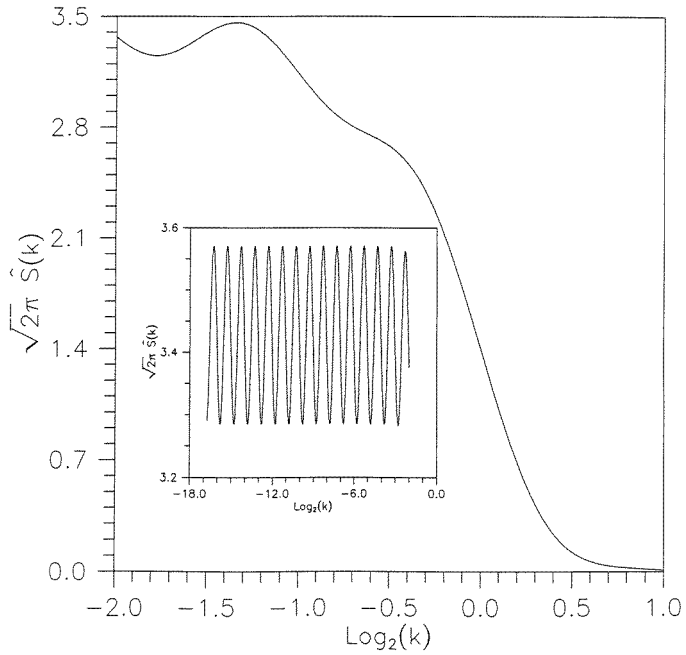

Figure 2. Log_2 plot of scaling function.

where $W\Psi(\rho^l,\, fa_0 j\rho^l + \delta_l[b]) = \frac{1}{\sqrt{\rho^l}} \int_{-\infty}^{+\infty} \mathrm{d}x\, \mathcal{W}_0(\frac{x-\{fa_0 j\rho^l+\delta_l[b]\}}{\rho^l})\Psi(x)$.

There are several variations on equation (3.19*b*) of interest to us. The first involves rewriting the argument of the $\mathcal{D}$ function according to $n_l[b] - j = \frac{n_l[b]\times\Delta_l+\delta_l[b]-j\times\Delta_l-\delta_l[b]}{\Delta_l}$ or $n_l[b] - j = \frac{b-j\times\Delta_l-\delta_l[b]}{\Delta_l} = \frac{b-jfa_0\rho^l-\delta_l[b]}{fa_0\rho^l}$. Substituting in equation (3.19*b*) yields

$$\Psi(b) = \frac{1}{\nu}\sum_{l=-\infty}^{+\infty}\sum_{j=-\infty}^{+\infty}\mathcal{D}\left(\frac{b - fa_0 j\rho^l - \delta_l[b]}{fa_0\rho^l}\right)\frac{1}{\sqrt{\rho^l}}W\Psi(\rho^l,\, fa_0 j\rho^l + \delta_l[b]). \tag{3.20}$$

If the wavelet transform is concentrated at sufficiently small scales, then the above expansion simplifies since $\mathrm{Lim}_{l\to-\infty}\delta[b] \to 0$ (and $\mathrm{Lim}_{l\to-\infty}n[b] \to \infty$). One then obtains the dyadic structure quoted in equation (1.9):

$$\Psi(b) \approx \frac{1}{\nu}\sum_{l=-\infty}^{+\infty}\sum_{j=-\infty}^{+\infty}W\Psi(\rho^l,\, fa_0 j\rho^l)\frac{1}{\sqrt{\rho^l}}\mathcal{D}\left(\frac{b - fa_0 j\rho^l}{fa_0\rho^l}\right). \tag{3.21}$$

Taking $fa_0 = 1$, $\rho = 2$, $\mathcal{W}_0(x) = -\mathcal{N}_h\partial_x^2\mathrm{e}^{-\frac{x^2}{2}}$ (i.e. $\hat{\mathcal{W}}_0(k) = \mathcal{N}_h k^2\mathrm{e}^{-\frac{k^2}{2}}$), and $\mathcal{D}(j) = -\mathcal{N}_h\partial_j^2\mathrm{e}^{-\frac{j^2}{2}}$, we recover the (approximate) dyadic expansion in equation (1.9).

Another possibility is to transform equation (3.19) into the form

$$\Psi(b) = \frac{1}{\nu}\sum_{l=-\infty}^{+\infty}\sum_{j=-\infty}^{+\infty}\mathcal{D}(j)\,\frac{1}{\sqrt{\rho^l}}W\Psi(\rho^l, b - fa_0 j\rho^l) \tag{3.22}$$

where $W\Psi(\rho^l, b - fa_0 j\rho^l) = \frac{1}{\sqrt{\rho^l}} \int_{-\infty}^{+\infty} \mathrm{d}x\, \mathcal{W}_0(\frac{x-\{b-fa_0 j\rho^l\}}{\rho^l})\Psi(x)$.

If Ψ corresponds to an atomic measure, $\Psi(x) = \sum_{i=1}^{I}\mathcal{A}_i\delta(x - \beta_i)$, with $\mu(p) = \int \mathrm{d}x\, x^p\Psi(x) = \sum_{i=1}^{I}\mathcal{A}_i(\beta_i)^p$, then the wavelet transform integral can be transformed into a superposition of dilated and translated versions of the derivatives of the mother wavelet expression:

$$\Psi(b) = \frac{1}{\nu}\sum_{l=-\infty}^{+\infty}\sum_{j=-\infty}^{+\infty}\sum_{p=0}^{+\infty}\frac{\mathcal{D}(j)\mu(p)}{\rho^{l(p+1)}p!}\mathcal{W}_0^{(p)}\left(\frac{fa_0 j\rho^l - b}{\rho^l}\right). \tag{3.23}$$

3.4. An alternative formulation

Returning to equation (3.11), we do not have to define our partition ending at $a_\infty = +\infty$. Instead, we can take $a_{+1} = +\infty$, and $a_l \to 0$, for l: $0 \to -\infty$. We can use the same formalism as before, taking $\rho_l = \frac{a_{l+1}}{a_l}$, for $l \leqslant -1$. Again, upon taking $\rho_l = \rho$, a constant, we obtain $a_l = a_0\rho^l$. The reconstruction formula in equation (3.22) would then become

$$\Psi(b) = \frac{1}{\nu}\left[\frac{1}{a_0}\int \mathrm{d}x\, \mathcal{S}\left(\frac{x-b}{a_0}\right)\Psi(x) + \sum_{l=-1}^{-\infty}\sum_{j=-\infty}^{+\infty}\frac{\mathcal{D}(j)}{\sqrt{\rho^l}}W\Psi(\rho^l, b - fa_0 j\rho^l)\right]. \tag{3.24}$$

4. A numerical example

We illustrate the MQ-DCWT formalism by applying it to the ground state of the quartic anharmonic oscillator problem defined by the potential $V(x) = mx^2 + gx^{2q}$, $q = 2$. The specific MQ formalism for this problem is presented within the general anharmonic oscillator problem ($q \geqslant 2$) formalism, for completeness. A fuller discussion is given elsewhere (HM 1998).

Table 1. Energy and missing moments.

$V(x)$	E	$\mu(l=0,2)$ ($\mu(\text{odd})=0$)
x^2+x^4	1.392 351 6415	0.642 670 6223
		0.357 329 3777

Translating the Schrödinger equation by 'b', and working with the configuration $\Phi_{\gamma,b}(x) \equiv \mathrm{e}^{-\gamma x^2}\Psi(x+b)$ (for the Mexican hat wavelet case), where $\gamma \equiv \frac{1}{2a^2}$, results in the differential equation

$$-[\partial_x^2 + 4\gamma x\partial_x + \{2\gamma + 4\gamma^2 x^2\}]\Phi_{\gamma,b}(x) + \left[m\{x^2+2bx+b^2\} + g\sum_{i=0}^{2q}\binom{2q}{i}b^{2q-i}x^i\right]\Phi_{\gamma,b}(x) = E\Phi_{\gamma,b}(x). \tag{4.1}$$

The power moments of interest are $\mu_{\gamma,b}(p) \equiv \int_{-\infty}^{\infty} \mathrm{d}x\, x^p \Phi_{\gamma,b}(x)$. Multiplying both sides of equation (4.1) by x^p and performing the necessary integration by parts, one obtains the moment equation

$$-p(p-1)\mu_{\gamma,b}(p-2) + [\gamma(4p+2) + mb^2 + gb^{2q} - E]\mu_{\gamma,b}(p) + [2bm + 2gqb^{2q-1}]\mu_{\gamma,b}(p+1) + [m - 4\gamma^2 + gq(2q-1)b^{2q-2}]\mu_{\gamma,b}(p+2) + g\sum_{i=3}^{2q-1}\binom{2q}{i}b^{2q-i}\mu_{\gamma,b}(p+i) + g\mu_{\gamma,b}(p+2q) = 0. \tag{4.2}$$

The missing moment order is $m_s = 2q-1$. One can then define the $M_{\gamma,b,E}(p,l)$ coefficients in equation (2.10), which must also satisfy equation (4.2) for fixed l, as well as the initialization conditions $M_{\gamma,b,E}(i,j) = \delta_{i,j}$ for $0 \leqslant i, j \leqslant m_s$.

For the quartic anharmonic problem, the ground state energy and missing moments $\mu_{\gamma=0,0}(l)$ were determined through the eigenvalue moment method of Handy, Bessis and co-workers (1988a, b). A recent generalization of it also facilitates the analysis of excited states (Handy 1999a). Another possible approach is to use the quantization methods in the work by Tymczak *et al* (1998a, b). As previously noted, all of these determine the energy and missing moments before the coupled moment equations (i.e. equation (1.2) or (4.3)) are integrated with respect to the inverse scale variable, γ. Alternatively, other recent methods use equation (4.3) directly in order to determine the energy and missing moments (Handy *et al* 1999, Handy 1999b).

We will assume in the following numerical analysis that the energy and missing moments have been determined prior to integrating equation (1.2). For the case of the quartic anharmonic oscillator, the relevant equations (analogous to equation (2.13)) become

$$\frac{\partial}{\partial\gamma}\begin{pmatrix}\mu_{\gamma,b}(0)\\ \mu_{\gamma,b}(1)\\ \mu_{\gamma,b}(2)\\ \mu_{\gamma,b}(3)\end{pmatrix} = \begin{pmatrix}0 & 0 & -1 & 0\\ 0 & 0 & 0 & -1\\ \mathcal{M}_{2,0}[\gamma] & \mathcal{M}_{2,1}[\gamma] & \mathcal{M}_{2,2}[\gamma] & \mathcal{M}_{2,3}[\gamma]\\ \mathcal{M}_{3,0}[\gamma] & \mathcal{M}_{3,1}[\gamma] & \mathcal{M}_{3,2}[\gamma] & \mathcal{M}_{3,3}[\gamma]\end{pmatrix}\begin{pmatrix}\mu_{\gamma,b}(0)\\ \mu_{\gamma,b}(1)\\ \mu_{\gamma,b}(2)\\ \mu_{\gamma,b}(3)\end{pmatrix}. \tag{4.3}$$

The specification of the matrix coefficients are given elsewhere (HM 1996).

In table 1 we quote the physical energy and missing moment values for the ground state of the quartic anharmonic oscillator. Utilizing these as initial values in the integration of equation (4.3), we can integrate the coupled moment equations up to any finite inverse scale ($\gamma < \infty$) and translation values ($-\infty < b < +\infty$). Note that equation (2.6) is implicitly used in determining the required $\mu_{\gamma=0,b}(p)$.

Table 2. Asymptotic estimates for $\Psi(b)$.

$\delta\gamma$	b	γ_s	$\sqrt{\frac{\gamma_s}{\pi}}\mu_{\gamma_s,b}(0)$	$\frac{2\gamma_s^{\frac{3}{2}}}{\sqrt{\pi}}\mu_{\gamma_s,b}(2)$	$\Psi_{\text{true}}(b)$
10^{-3}	0	26	0.322	0.314	0.325
	1	25	0.152	0.154	0.151
	2	24	0.839(−2[a])	0.112(−1)	0.705(−2)
	3	23	0.143(−4)	0.364(−4)	0.610(−5)
	4	30	0.376(−6)	0.677(−5)	
10^{-4}	0	84	0.325	0.323	0.325
	1	83	0.151	0.152	0.151
	2	82	0.742(−2)	0.822(−2)	0.705(−2)
	3	81	0.777(−5)	0.117(−4)	0.610(−5)
	4	29	0.462(−6)	0.506(−5)	
10^{-5}	0	200	0.326	0.325	0.325
	1	200	0.151	0.151	0.151
	2	200	0.717(−2)	0.751(−2)	0.705(−2)
	3	200	0.665(−5)	0.808(−5)	0.610(−5)
	4	30	0.390(−6)	0.440(−5)	

[a] To the power of ten.

Knowledge of the moments allows us to determine the Mexican hat wavelet transform for scale and translation values required in any of the DCWT reconstruction formulae cited in section 3.2 (i.e. equations (3.19)–(3.24)). The specific reconstruction procedure adopted here utilizes the Mexican hat wavelet and dual function expressions $\mathcal{W}_0(x) = -\mathcal{N}_h\partial_x^2 e^{-\frac{x^2}{2}} = \mathcal{N}_h(x^2-1)e^{-\frac{x^2}{2}}$, $\mathcal{D}(j) = \mathcal{N}_j(j^2-1)e^{-\frac{j^2}{2}}$, respectively ($\mathcal{N}_h = \frac{2}{\sqrt{3\sqrt{\pi}}}$), for dyadic parameter values, $\rho = 2$, $fa_0 = 1$. The Mexican hat wavelet transform is given by

$$W\Psi(a(\gamma),\xi) = (2\gamma)^{\frac{1}{4}}\mathcal{N}_h(\mu_{\gamma,\xi}(0) - 2\gamma\mu_{\gamma,\xi}(2)). \tag{4.4}$$

Two important relations are the asymptotic expressions (i.e. equation (2.14))

$$\text{Lim}_{\gamma\to\infty}\sqrt{\frac{\gamma}{\pi}}\mu_{\gamma,b}(0) = \Psi(b) \tag{4.5a}$$

and

$$\text{Lim}_{\gamma\to\infty}\frac{2\gamma^{\frac{3}{2}}}{\sqrt{\pi}}\mu_{\gamma,b}(2) = \Psi(b). \tag{4.5b}$$

We can integrate equation (4.3) using Runge–Kutta (RK) methods. In table 2 we compare both asymptotic estimates for $\Psi(b)$, for various RK step sizes, $\delta\gamma$.

For a given $\delta\gamma$ (the RK integration step), the RK integration with respects to γ, for fixed b, became unstable for γ values beyond those cited in table 2 (with the exception of the $\gamma = 200$ values quoted). From equation (3.22), at a given b value, we want to sum over the DCWT terms, $W\Psi(2^l, b - j2^l)$, for which the scale and translation values ($a = 2^l$, $\xi = b - j2^l$, respectively) are within the numerical stability region of our RK integration. As $l \to +\infty$ ($a_l \to \infty$, $\gamma_l \to 0$), our RK analysis suggests that ξ can be arbitrary. However, as $l \to -\infty$ ($a_l \to 0$, $\gamma_l \to \infty$), then the results in table 2 limit the translation values accordingly. In figure 3 we compare the true ground state solution (normalized according $\Psi(0) = 0.325$, Handy and Murenzi (1996)) with the expansion in equation (3.22). The 'l' and 'j' summation indices were chosen to be consistent with the aforementioned numerical stability requirements as well as: $-10 \leqslant l \leqslant 30$ and $|j2^l| \leqslant 5$. Also, $\delta\gamma = 10^{-4}$. The numerical results are satisfactory and validate our formalism.

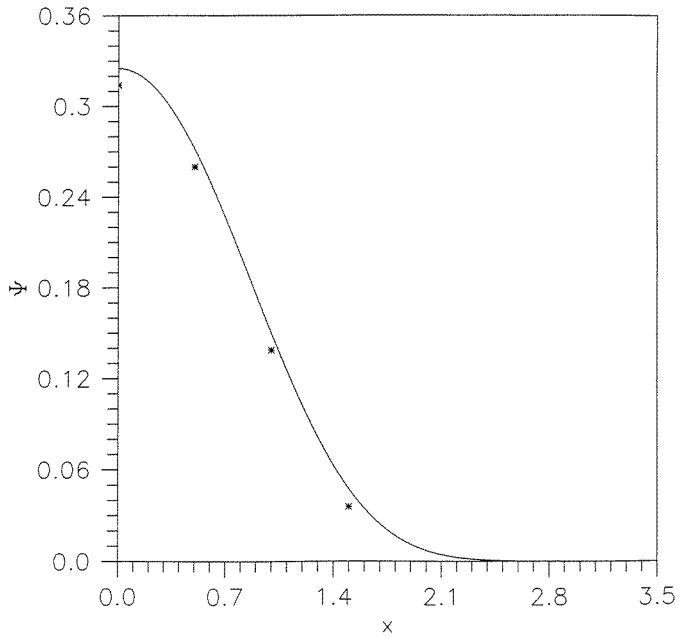

Figure 3. DCWT approximation of ground state: $-\partial^2\Psi(x) + (x^2 + x^4)\Psi(x) = E\Psi(x)$.

5. Conclusion

We have shown how MQ naturally leads to an exact (A-adic) discrete–continuous wavelet formulation for reconstructing the wavefunction corresponding to arbitrary, one-dimensional, rational fraction potential functions.

Acknowledgments

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Appendix. (Analysis of equation (3.18))

As noted in section 3, the relations in equations (3.18a), (3.18b) constrain the three functions $\hat{\mathcal{S}}(k)$, $\hat{\mathcal{W}}_0(k)$, and $\hat{\Upsilon}(k) \equiv \sum_{j=-\infty}^{\infty} \mathcal{D}(j)\mathrm{e}^{\mathrm{i}fjk}$, which are periodic. Acceptable choices for $\hat{\mathcal{W}}_0$ and $\mathcal{D}(j)$ must generate a scaling function, $\mathcal{S}(x)$, whose zeroth moment is nonzero, $\nu = \int \mathrm{d}x\, \mathcal{S}(x) \neq 0$, and otherwise well behaved (i.e. integrable, Fourier transformable, etc). We shall be working with $\rho = 2$, $f = a_0 = 1$, $\mathcal{D}(j) = -\mathcal{N}_h\partial_j^2\mathrm{e}^{-\frac{j^2}{2}} = \mathcal{N}_h(1 - j^2)\mathrm{e}^{-\frac{j^2}{2}}$, and $\mathcal{W}_0(x) = -\mathcal{N}_h\partial_x^2\mathrm{e}^{-\frac{x^2}{2}}$ or $\hat{\mathcal{W}}_0(k) = \mathcal{N}_h k^2\mathrm{e}^{-\frac{k^2}{2}}$. Recall that $\hat{\mathcal{R}}(k) \equiv \hat{\Upsilon}(k)\hat{\mathcal{W}}_0(k)$.

For future reference, under the above conditions, $|\hat{\Upsilon}(k)| < \sum_j |D(j)| < \infty$. Also,

$$W_S(k) \equiv \sum_{j=0} \hat{\mathcal{W}}_0(\rho^j k) = \mathcal{N}_h k^2 \sum_{j=0} (\rho^2)^j \mathrm{e}^{-\frac{1}{2}(k\rho^j)^2} \tag{A.1}$$

converges, for $k \neq 0$, by the ratio test (i.e. $\exp(-\frac{1}{2}k^2[\rho^2 - 1]\rho^{2j}) \to 0$, as $j \to \infty$). Furthermore, $\mathrm{Lim}_{k\to\infty} W_S(k) = 0$, since for a sufficiently large J, and $j \geqslant J$, we have $\rho^{2j} \geqslant 2j\rho + C_J$, for the positive constant $C_J = \rho^{2J} - 2J\rho$. This then yields

$$W_S(k) < \mathcal{N}_h k^2 \left(\sum_{j=0}^{J-1} (\rho^2)^j \mathrm{e}^{-\frac{1}{2}(k\rho^j)^2} + \sum_{j=J} (\rho^2)^j \mathrm{e}^{-\frac{1}{2}(k^2[2j\rho + C_J])} \right) \tag{A.2a}$$

or

$$W_S(k) < \mathcal{N}_h k^2 \left(\sum_{j=0}^{J-1} (\rho^2)^j \mathrm{e}^{-\frac{1}{2}(k\rho^j)^2} + \rho^{2J} \frac{\mathrm{e}^{-\frac{1}{2}k^2(C_J + 2\rho J)}}{1 - \rho^2 \mathrm{e}^{-\rho k^2}} \right) \tag{A.2b}$$

provided $\rho^2 \mathrm{e}^{-\rho k^2} < 1$.

Consider the infinite sequence of points $k_* \rho^i$, for $i \in (-\infty, +\infty)$, and $k_* \in (1, \rho]$. Clearly, all points along the positive k-axis can be related to some i and k_* value. Taking $\sigma_i \equiv \hat{\mathcal{S}}(k_* \rho^i)$ (where σ_0 is arbitrary), we obtain

$$\sigma_{i+1} = \sigma_i - \hat{\mathcal{R}}(k_* \rho^i). \tag{A.3}$$

Thus, knowledge of $\sigma_{+\infty}$ determines all the σ_i values. We shall return to this in equation (A.8*b*).

If we assume $\hat{\mathcal{R}}(k)$ is continuous at $k = 0$, then equation (A.3) becomes (approximately) $\sigma_{i+1} \approx \sigma_i - \hat{\mathcal{R}}(0)$ which leads to the asymptotic limit $\sigma_i = c(k_*) - (\hat{\mathcal{R}}(0))i$, as $i \to -\infty$. Therefore, to avoid unbounded solutions, we require that

$$\hat{\mathcal{R}}(0) = \hat{\Upsilon}(0)\hat{\mathcal{W}}_0(0) = 0. \tag{A.4}$$

The general solution to equation (3.18*a*) is of the form

$$\hat{\mathcal{S}}(k) = \hat{\Omega}(k) + \hat{\mathcal{P}}(k) \tag{A.5}$$

where $\hat{\Omega}(k) = \sum_{i=0}^{\infty} \hat{\mathcal{R}}(\rho^i k)$ and $\hat{\mathcal{P}}(k) = \sum_{n=-\infty}^{+\infty} c_n \mathrm{e}^{2\pi \mathrm{i} \frac{\ln(k)}{\ln(\rho)}}$, is an arbitrary, geometrically periodic function, $\hat{\mathcal{P}}(k) = \hat{\mathcal{P}}(\rho k)$ ($\rho > 1$). Note that $\hat{\mathcal{P}}(k)$ is the general homogeneous solution to equation (3.18*a*) (corresponding to an arbitrary, conventionally periodic solution in the variable $\ln(k)$, with period $\ln(\rho)$).

Through the analysis presented in the context of equations (A.1)–(A.2*b*) one can argue that $\hat{\Omega}(k)$ exists and is asymptotically zero, as $k \to \infty$. Since it corresponds to a special solution to equation (3.18*a*), it will be geometrically periodic at the origin (with infinite derivatives),

$$\mathrm{Lim}_{l\to\infty}(\hat{\Omega}(k\rho^{-(l+1)}) - \hat{\Omega}(k\rho^{-l})) = 0 \tag{A.6}$$

as well as discontinuous at $k = 0$, despite the fact that $\hat{\mathcal{R}}(0) = 0$.

Just as $\hat{\Omega}(k)$ becomes nondifferentiable as $k \to 0$, so too will the general homogeneous solution $\hat{\mathcal{P}}(k)$ (other than the trivial constant solution). However, it is possible to combine both to produce a special analytic solution.

If we conjecture $\hat{\mathcal{S}}(k)$ to be analytic, then it is uniquely determined, up to a constant. In this case, $\hat{\mathcal{R}}(k)$ is also analytic. Let

$$\hat{\mathcal{S}}(k) = \frac{1}{\sqrt{2\pi}} \sum_{n \geqslant 0} \frac{\nu(n)}{n!} (-\mathrm{i}k)^n \tag{A.7a}$$

and

$$\hat{\mathcal{R}}(k) \equiv \frac{1}{\sqrt{2\pi}} \sum_{n=0}^{\infty} \tau_n (-\mathrm{i}k)^n \tag{A.7b}$$

then

$$[1 - \rho^n] \frac{\nu(n)}{n!} = \tau_n. \tag{A.7c}$$

Note that self-consistency requires $\hat{\mathcal{R}}(0) = \frac{1}{\sqrt{2\pi}}\tau_0 = 0$. Furthermore, $\nu(0)$ is undetermined and arbitrary. Application of the ratio test readily shows that the radius of convergence for $\hat{\mathcal{S}}(k)$ is determined by that for $\hat{\mathcal{R}}(k)$ since $\frac{\rho}{n+1}\frac{\nu(n+1)}{\nu(n)} \to \frac{\tau_{n+1}}{\tau_n}$, as $n \to +\infty$.

Denoting this special (up to an arbitrary constant) analytic solution by $\hat{\mathcal{S}}_a(k)$, it must be representable in terms of the general solution given in equation (A.5), $\hat{\mathcal{S}}_a(k) = \hat{\Omega}(k) + \hat{\mathcal{P}}_s(k)$, for a special geometrically periodic configuration, $\hat{\mathcal{P}}_s(k)$, capable of smoothing out the infinite oscillations, at the origin, exhibited by $\hat{\Omega}(k)$. Since $\hat{\Omega}(k) \to 0$, as $k \to \infty$, then $\hat{\mathcal{S}}_a(k)$ becomes geometrically periodic at infinity and nonzero.

Clearly, from the entire preceding analysis, the only special solution is the one corresponding to

$$\mathrm{Lim}_{k\to+\infty}\hat{\mathcal{S}}(k) \to 0 \tag{A.8a}$$

as defined by $\hat{\Omega}$. In terms of the iterative representation in equation (A.3), we have

$$\mathrm{Lim}_{i\to+\infty}\sigma_i = 0. \tag{A.8b}$$

This means that we will be taking

$$\hat{\mathcal{S}}(k) = \sum_{i=0}^{+\infty}\hat{\mathcal{R}}(\rho^i k). \tag{A.9}$$

We can generate this solution directly from equation (A.9) (which would entail two series summations, one for generating $\hat{\mathcal{R}}$, the other for generating equation (A.9)), or through a numerical iteration based on equation (A.8*b*). We adopted the latter, as explained below. Note that $\hat{\mathcal{S}}(k) = \hat{\mathcal{S}}(-k)$ (because $\hat{\mathcal{R}}(k) = \hat{\mathcal{R}}(-k)$ and equation (3.18*a*)).

The zeroth moment of the scaling function, $\nu(0)$, is required in any signal-wavelet reconstruction formulation. The special $\hat{\mathcal{S}}(k)$ solution being considered has an inverse Fourier transform (i.e. because $\hat{\mathcal{S}}(k)$ is asymptotically bounded), $\mathcal{S}(x)$. However, because $\hat{\mathcal{S}}(k)$ is not analytic at the origin (due to its geometrically periodic nature), we cannot determine $\mathcal{S}$'s zeroth moment from the usual relation ($\nu(0) \neq \sqrt{2\pi}\hat{\mathcal{S}}(0)$). Neither can we take $\nu(0) = \sqrt{2\pi}\mathrm{Lim}_{\epsilon\to0}(\frac{1}{2\epsilon}\int_{-\epsilon}^{+\epsilon}\mathrm{d}k\,\hat{\mathcal{S}}(k))$, since $\nu_\epsilon = \frac{1}{2\epsilon}\int_{-\epsilon}^{+\epsilon}\mathrm{d}k\,\hat{\mathcal{S}}(k)$ would be geometrically periodic as well, and not have a limit as $\epsilon \to 0^+$. To see this, consider any geometrically periodic function, $\hat{\mathcal{P}}(k)$. Let $\epsilon = k_0\rho$, then $\nu_\epsilon[\hat{\mathcal{P}}] = \sqrt{2\pi}\frac{\sum_{i=0}^{\infty}\rho^{-i}\alpha}{\sum_{i=0}^{\infty}\rho^{-i}\lambda} = \sqrt{2\pi}\frac{\alpha}{\lambda}$, where $\alpha = \int_{k_0}^{\rho k_0}\mathrm{d}k\,\hat{\mathcal{P}}(k)$, and $\lambda = k_0(\rho-1)$. Accordingly, $\nu_{\epsilon(k_0)}[\hat{\mathcal{P}}] = \frac{\sqrt{2\pi}}{\rho-1}\int_1^\rho \mathrm{d}k\,\hat{\mathcal{P}}(k_0k)$, which is geometrically periodic in k_0, with geometric period ρ.

We are then forced to take the logarithmic average

$$\nu(0) = \sqrt{2\pi}\mathrm{Lim}_{\epsilon\to0}\frac{\int_\epsilon^\Lambda \frac{\mathrm{d}k}{k}\hat{\mathcal{S}}(k)}{\int_\epsilon^\Lambda\frac{\mathrm{d}k}{k}} \tag{A.10a}$$

or

$$\nu(0) = \sqrt{2\pi}\mathrm{Lim}_{\ln(\epsilon)\to-\infty}\frac{\int_{\ln(\epsilon)}^{\ln(\Lambda)}\mathrm{d}\xi\,\hat{\mathcal{S}}(\mathrm{e}^\xi)}{\int_{\ln(\epsilon)}^{\ln(\Lambda)}\mathrm{d}\xi} \tag{A.10b}$$

for arbitrary Λ. This is equal to

$$\nu(0) = \sqrt{2\pi}\mathrm{Lim}_{\epsilon\to0}\frac{\int_{\ln(\epsilon)-\ln(\rho)}^{\ln(\epsilon)}\mathrm{d}\xi\,\hat{\mathcal{S}}(\mathrm{e}^\xi)}{\ln(\rho)}. \tag{A.10c}$$

The justification for taking the logarithmic average is as follows. Consider defining the zeroth moment of the inverse Fourier transform function, $\mathcal{S}(x)$, in terms of a limiting process ($\epsilon \to 0$) for the integral

$$\int_{-\infty}^{+\infty}\mathrm{d}x\,R^*_{\epsilon,\Lambda}(x)\mathcal{S}(x) = \int_{-\infty}^{+\infty}\mathrm{d}k\,\hat{R}^*_{\epsilon,\Lambda}(k)\hat{\mathcal{S}}(k) \tag{A.11}$$

where $\hat{\mathcal{S}}(k) = \hat{\mathcal{S}}(-k)$ and $\hat{R}_{\epsilon,\Lambda}(k) = \hat{R}_{\epsilon,\Lambda}(-k)$. Let

$$\hat{R}_{\epsilon,\Lambda}(k) = \begin{cases} 0 & |k| < \epsilon \\ \dfrac{\sqrt{\frac{\pi}{2}}}{\ln(\frac{\Lambda}{\epsilon})|k|} & \epsilon \leqslant |k| \leqslant \Lambda \\ 0 & |k| > \Lambda. \end{cases} \tag{A.12}$$

This reproduces equation (A.10*a*). We now show that $R_{\epsilon,\Lambda}(x)$ becomes unity in the $\epsilon \to 0$ limit.

The regulating function $R_{\epsilon,\Lambda}(x)$ is given by the inverse Fourier transform integral

$$R_{\epsilon,\Lambda}(x) = \frac{1}{\sqrt{2\pi}} \int \mathrm{d}k\, \mathrm{e}^{\mathrm{i}xk} \hat{R}_{\epsilon,\Lambda}(k) \tag{A.13a}$$

which becomes

$$R_{\epsilon,\Lambda}(x) = \frac{1}{\ln(\frac{\Lambda}{\epsilon})} \mathrm{Re}\left(\int_{\epsilon}^{\Lambda} \mathrm{d}k\, \frac{\mathrm{e}^{\mathrm{i}xk}}{k} \right). \tag{A.13b}$$

This expression is related to the exponential integral (i.e. Abramowitz and Stegun 1972). Clearly, $R_{\epsilon,\Lambda}(0) = 1$, and $\mathrm{Lim}_{x\to\infty} R_{\epsilon,\Lambda}(x) = 0$. As $\epsilon \to 0$, $R_{\epsilon,\Lambda}(x) \to 1$ since

$$R_{\epsilon,\Lambda}(x) = \frac{1}{\ln(\frac{\Lambda}{\epsilon})} \mathrm{Re}\left(\int_{1}^{\frac{\Lambda}{\epsilon}} \mathrm{d}k\, \frac{\mathrm{e}^{\mathrm{i}x\epsilon k}}{k} \right) \tag{A.14}$$

yields the expansion

$$R_{\epsilon,\Lambda}(x) = 1 + \frac{1}{\ln(\frac{\Lambda}{\epsilon})} \left(\sum_{n=2,4,\ldots} \frac{(-1)^{\frac{n}{2}} x^n}{n!n} (\Lambda^n - \epsilon^n) \right). \tag{A.15}$$

For the specific case being considered here (i.e. $\rho = 2$, $a_0 = f = 1$, $\mathcal{D}(j) = \mathcal{N}_h(1 - j^2)\mathrm{e}^{-\frac{j^2}{2}}$, and $\hat{\mathcal{W}}_0(k) = \mathcal{N}_h k^2 \mathrm{e}^{-\frac{k^2}{2}}$), figures 1 and 2 show the estimates for $\sigma_{i\to-\infty}(k_*)$, according to the numerical procedure previously suggested. That is, upon choosing $k_* \in (1, 2]$, we determined the $\hat{\mathcal{S}}(k_*)$ value satisfying equations (A.8*a*), (A.8*b*), for $0 \leqslant i < +\infty$. Using this $\hat{\mathcal{S}}(k_*)$ value, we recursively generate σ_i backwards, corresponding to $i \to -\infty$. The limiting values of this procedure are given in the cited figures. The bounded, oscillatory, nature of $\hat{\mathcal{S}}(k)$ (corresponding to equation (A.9)) is immediate. Using equation (A.10*c*), the value $\nu \approx 3.427$ is obtained, which compares well with Daubechies' estimate of $\frac{6.819}{2} = 3.410$ as given in equation (1.9).

References

Abramowitz M and Stegun I A (ed) 1972 *Handbook of Mathematical Functions* (New York: Dover)

Antoine J P, Vandergheynst P, Bouyoucef K and Murenzi R 1995 *Proc. SPIE* **2488** 486

Bender C M and Orszag S A 1978 *Advanced Mathematical Methods for Scientists and Engineers* (New York: McGraw-Hill)

Blankenbeckler R, De Grand T and Sugar R L 1980 *Phys. Rev.* D **21** 1055

Chui C K 1992 *An Introduction to Wavelets* (New York: Academic)

Daubechies I 1988 *Commun. Pure Appl. Math.* **41** 909

——1991 *Advances in Spectrum Analysis and Array Processing* vol 1, ed S Haykin (Englewood Cliffs, NJ: Prentice Hall)

Grossmann A and Morlet J 1984 *SIAM J. Math. Anal.* **15** 723

Handy C R 1981 *Phys. Rev.* D **24** 378

——1999a Quasi-positivity and moment quantization *CAU Preprint*

——1999b Scalets, wavelets, and turning point quantization *CAU Preprint*

Handy C R and Bessis D 1985 *Phys. Rev. Lett.* **55** 931

Handy C R, Bessis D and Morley T D 1988b *Phys. Rev.* A **37** 4557
Handy C R, Bessis D, Sigismondi G and Morley T D 1988a *Phys. Rev. Lett.* **60** 253
Handy C R and Murenzi R 1996 *Phys. Rev.* A **54** 3754
——1997 *J. Phys. A: Math. Gen.* **30** 4709
——1998a *J. Phys. A: Math. Gen.* **31** 9897
——1998b *Phys. Lett.* A **248** 7
——1999 *Proc. 1996 Montreal Workshop on Spline Functions and the Theory of Wavelets* ed S Dubuc and G Deslauriers (Providence, RI: American Mathematical Society)
Handy C R, Murenzi R, Bouyoucef K and Brooks H A 1999 *CAU Preprint*
Killingbeck J P, Jones M N and Thompson M J 1985 *J. Phys. A: Math. Gen.* **18** 793
Paul T 1984 *J. Math. Phys.* **25** 3252
Plantevin F 1992 Une application de la transformée en ondelettes continue à la mécanique quantique et analyse multi-résolution adaptive *PhD Thesis* Université de Provence
Tymczak C J, Japaridze G S, Handy C R and Wang Xiao-Qian 1998a *Phys. Rev. Lett.* **80** 3673
——1998b *Phys. Rev.* A **58** 2708
Tymczak C J and Wang Xiao-Qian 1997 *Phys. Rev. Lett.* **78** 3654